Name: ____________________, ____________________

PHYSICS 619 : SPRING SEMESTER 2019

Project #11: Path-Integral Monte Carlo

1) We want to solve for the ground state of the dimensionless harmonic oscillator Hamiltonian operator

$$\hat{H} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2,$$

by the path-integral Monte Carlo method. In class, we have shown that the second-order propagator is given by (with $V(x) = \frac{1}{2}x^2$)

$$G_2(x, x'; \Delta\tau) = \frac{1}{\sqrt{2\pi\Delta\tau}} \exp[-\frac{1}{2\Delta\tau}(x - x')^2] \exp[-\frac{1}{2}\Delta\tau(V(x) + V(x'))] = \mathrm{e}^{-S_2(x,x';\Delta\tau)}$$

where the second-order action is given by (can ignore the first, constant term for now)

$$S_2(x, x'; \Delta\tau) = \frac{1}{2}\ln(2\pi\Delta\tau) + \frac{1}{2\Delta\tau}(x - x')^2 + \frac{1}{2}\Delta\tau(V(x) + V(x')).$$

What is the local energy function

$$E_L(x, x'; \Delta\tau) = \frac{\hat{H}G_2(x, x'; \Delta\tau)}{G_2(x, x'; \Delta\tau)}?$$

2) For $\tau = 1$ to 10 in increments of 0.5, take $\Delta\tau = \tau/2$ and generate a set of $\{x_1, x_2\}$ by the Metropolis algorithm according to

$$\begin{aligned} p(x_1, x_2) &\propto G_2(x_1, x_2; \Delta\tau)G_2(x_2, x_1; \Delta\tau) \\ &\propto \exp(-S(x_1, x_2)) \end{aligned}$$

where the 2-bead action is given by

$$S(x_1, x_2) = S_2(x_1, x_2; \Delta\tau) + S_2(x_2, x_1; \Delta\tau),$$

and compute the 2-bead energy expectation values (take $n = 10^6$)

$$\langle E_L \rangle = \frac{1}{n}\sum_{i=1}^{n} \frac{1}{2}[E_L(x_{1i}, x_{2i}; \Delta\tau) + E_L(x_{2i}, x_{1i}; \Delta\tau)].$$

Plot $\langle E_L \rangle$ vs τ and compare it to the analytical result $1/2 + \mathrm{e}^{-\tau}/(1 - \mathrm{e}^{-\tau})$.

3) Repeat the above for a 4-bead calculation, *i.e.*, for $\tau = 1$ to 10, in increments of 0.5, take $\Delta\tau = \tau/4$ and generate a set of $\{x_1, x_2, x_3, x_4\}$ by the Metropolis algorithm according to

$$\begin{aligned} p(x_1, x_2, x_3, x_4) &\propto G_2(x_1, x_2; \Delta\tau)G_2(x_2, x_3; \Delta\tau)G_2(x_3, x_4; \Delta\tau)G_2(x_4, x_1; \Delta\tau) \\ &\propto \exp(-S(x_1, x_2, x_3, x_4)) \end{aligned}$$

where the 4-bead action is now given by

$$S(x_1, x_2, x_3, x_4) = S_2(x_1, x_2; \Delta\tau) + S_2(x_2, x_3; \Delta\tau) + S_2(x_3, x_4; \Delta\tau) + S_2(x_4, x_1; \Delta\tau).$$

Plot the 4-bead energy expectation values (take $n = 10^6$)

$$\langle E_L \rangle = \frac{1}{n}\sum_{i=1}^{n} \frac{1}{4}[E_L(x_{1i}, x_{2i}; \Delta\tau) + E_L(x_{2i}, x_{3i}; \Delta\tau) + E_L(x_{3i}, x_{4i}; \Delta\tau) + E_L(x_{4i}, x_{1i}; \Delta\tau)].$$

as a function of τ in the same graph as in 2).

4. (10 pt bonus) Do the 8-bead case and plot the result in the same graph. Note that by explicitly summing the action or the local energy, you may get a more compact analytical expression. The forms used above are for conceptional clarity. Textbook PIMC which does not use the Hamiltonian estimator above, gives no recognizable results for small number of beads.